

TRANSMUTING COPPER INTO A MAIN GROUP ELEMENT

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A vast number of chemical reactions rely on the near-inevitable preference of copper for positive oxidation states to make useful compounds. Recently, we have isolated a stable compound with a copper-magnesium bond,^[1] which conforms to the formal oxidation state of Cu(-I). Quantum chemical calculations further support the assignment of a low charge at copper (QTAIM: $q_{\text{Cu}} = -0.52$, $q_{\text{Mg}} = +1.45$), and NPA shows a $3d^{10}4s^{1,2}$ electronic configuration at copper, an electronic transmutation of copper away from the d-block and into the main group.

Since our initial report, we have recorded X-ray absorption spectroscopy data for our CuMg complex, which showed a copper K-edge energy of 8979.6 eV. These data, combined with measurements on 13 reference compounds, and additional computational investigations now allow us to report a clearer understanding of the nature of the CuMg interaction.

The CuMg bond acts as a source of the cupride anion, transferring the NHC-copper fragment to electrophilic s-, p-, and d-block atoms to make known and new copper-containing compounds, such as a complex with an unsupported CuZn bond. We can now access copper-element bonds a much wider swathe of the periodic table.

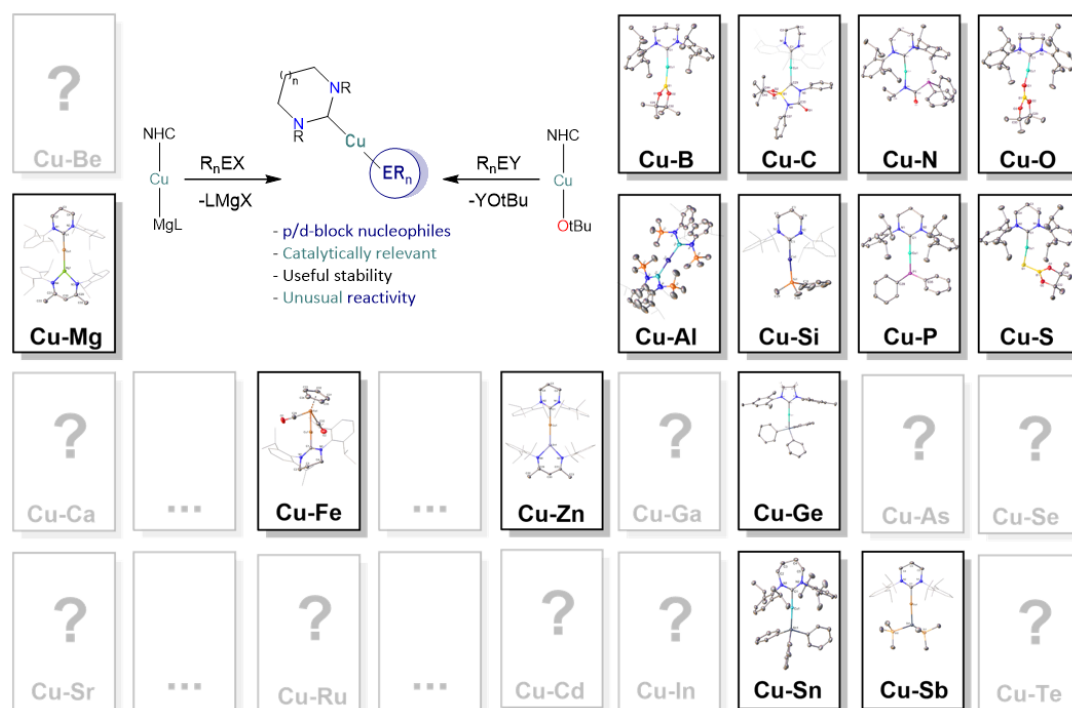


Figure 1 A summary of our exploration into copper-element bonds.

[1] R. A. Jackson, N. J. Evans, D. J. Babula, T. M. Horsley Downie, R. S. C. Charman, S. E. Neale, M. F. Mahon, and D. Liptrot, *Nature Communications*, 2025, 16, 110